demands compulsorily the following equalities:
\[ h_4 = h_2; \ h_5 = h_3; \ k_5 = k_3; \ k_4 = k_2. \]

Only in this case the lines possess indices:
\[ a_1 = (h_1k_10); \ a_2 = (h_2k_20); \ a_3 = (h_3k_30). \]

The machine puts into ‘memory’ the numbers \( P \), satisfying the criterion of simultaneity.

Further one takes the triplet of numbers \( a_1, a_2, a_4 \) and carries out all the above calculations for it. The process is repeated for \( a_1, a_2, a_5 \) and \( a_1, a_2, a_6 \) and so on as far as the triplet of numbers \( a_{n-2}, a_{n-1}, a_n \). The program is analogous for the other \( D \)-expressions from Table 2.

The application of this method to the indexing of the X-ray pattern lines of all the systems will be shown in a subsequent paper, and as is already seen the partial indexing of lines takes place in the process of identification of the system, as the definite indices of interference are put in correspondence to three selected lines.

From our point of view, the ‘constant parameters method’ possesses the following basic advantages in comparison with the method of Runge and Ito. First, according to theoretical and practical estimates this method can work at a larger absolute error in the determination of the Wolf-Bragg angle:
\[ \Delta \theta_{\text{const.\,param.}} \approx 10^2 \Delta \theta_{\text{Ito}}. \]

Consequently, if \( \Delta Q_{\text{hkl}} \approx 10^{-3} \cdot Q_{\text{hkl}} \) is necessary in Ito’s method, it is sufficient to have \( \Delta Q_{\text{hkl}} \approx 10^{-2}Q_{\text{hkl}} \) in the constant parameters method. Secondly, this method is simpler in programming than the Runge–Ito method.

The systems of two already known substances (NiAl3, orthorhombic – 12 lines – and Zr, hexagonal – 14 lines) have been determined as a check and to perfect the technique of the method. The calculations by the suggested method were carried out on a BECM-4 computer. The results are in complete agreement with expectations.

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References


**The Intensity Distribution and Variance of the Iron Kα Multiplet**

**By H. J. Edwards and K. Toman***

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*(Received 21 May 1969)*

The variance of the Kα12 doublet of iron X-radiation as a function of truncation range was determined using a silicon analysing crystal. The presence of satellite lines gives rise to an initial ‘pseudolinear’ part to the variance–range curve; the origin and significance of this part are discussed. The effect of the satellite group was removed by interpolation of the line profile. The possibility of locating the background level by computation is investigated; it is shown that a mis-setting in the background level has an appreciable effect on the variance function, whilst a mis-setting in the background slope has negligible effect on the slope of the variance function. Results for both filtered and unfiltered radiation are given.

### 1. Introduction

There is a vast number of papers discussing the correlation between the variance of the powder diffraction profile and the state of the crystal – see the bibliography in Wilson (1963). The absolute practical application of the variance method depends on the knowledge of the variance of the spectral distribution of the radiation used. The variance for the Cu Kα doublet was determined by Langford (1968), but, so far as we know, this is the only radiation for which the variance has been experimentally determined.

The object of this paper is to give the dependence of the variance of the Fe Kα doublet on the truncation-range parameter \( \sigma \) and to discuss the influence of the location of the level of background on the resulting value of the intercept and slope of the variance function. Moreover, attention is paid to the effect of the group of satellite lines.

### 2. Spectral measurements

Spectral measurements were performed on an automatic Picker powder diffractometer. A silicon plate was used as the analysing crystal; its frontal plane was inclined at 0·5° to the atomic planes. The primary beam was limited in the equatorial plane by a slit 5 × 10⁻⁴ inch (0·013 mm) wide and the receiving slit was 10⁻³ inch...
(0.026 mm) wide. The distances from the limiting slit and the receiving slit to the crystal were 3.0 and 5.7 inch respectively. Between the crystal and the receiving slit a Soller slit with aperture 2° ($\Delta = 1^\circ$) was placed. No Soller slit was used in the primary beam. The X-ray tube was Dunlee type DZ–1B and was operated at 12mA and 28kV from the stabilized Picker source. A scintillation counter coupled with a pulse-height amplitude analyser was used as the detector.

The final measurements were made on the 333 reflexion of silicon. Preliminary measurements were also made on the 111 reflexion of silicon, the 200 and 400 reflexions of lithium fluoride, and the 101, 202 and 303 reflexions of $\alpha$ quartz, but the contribution of the instrumental aberrations to the intercept of the variance–range function and the contribution of the crystal function to the slope of the variance–range function were negligible only for the 333 reflexion of silicon. The results of the preliminary measurements were thus less satisfactory, but do not conflict with those presented here. An angular range of $\pm 3.5^\circ (\theta)$ about the centroid of the 333 reflexion was used. The number of recorded impulses per time unit at the peak of the $\alpha_1$ line slightly surpassed $9 \times 10^5$ and at the endpoints of the interval 900 and 1400 counts were recorded. The natural background (with X-ray window shut) was 130. The measurement was performed by the point-by-point technique with the step 0.02°(2$\theta$) long. To locate the background level with higher reliability, the intensity at additional points, $\pm 7.5^\circ (2\theta)$ and $\pm 11.5^\circ (2\theta)$, from the centroid was taken. The time unit was 700 sec for each point of the profile and 3500 sec for each additional background point.

In addition to this measurement, which was carried out without a $\beta$ filter, another run was performed with filtered radiation. The attenuation of the Mn foil was 2.6 for the $\alpha_1$ line, the counting time was 980 sec for ordinary points and 4900 sec for the extra points in the background. These background measurements were performed at points $+ 7.5^\circ (\theta)$ and $+ 11.5^\circ (\theta)$ from the centroid. Points at the high-energy side ($- 7.5^\circ$ and $- 11.5^\circ$) were omitted, because they were beyond the absorption edge.

In Fig. 1, the result of the measurement without the $\beta$ filter is recorded. In addition to the lines $\alpha_1$ and $\alpha_2$ of the $K\alpha$ doublet, the Figure shows the satellite group. The width of the $\alpha_1$ line is 0.86 mA (measured at half peak height); its asymmetry coefficient is 0.23 (defined as $(W_- - W_+)/(W_+ + W_-)$ where $W_-$ is the high-energy half width measured from the peak, and $W_+$ is the corresponding low-energy half width). The width of the $\alpha_2$ line is 1.02 mA and its asymmetry is 0.10. The distance of the centre of the satellite group from the common centroid is 10.0 mA and its half width is 2.7 mA. This means that the satellite group influences the intensity distribution at least from 7.8 to 12.2 mA on the high-energy side of the doublet (measured from the centroid). A future paper by J.I. Langford will discuss the spectroscopy of the $K\alpha$ and $K\beta$ lines of iron.

3. The computation of the variance

The computation of the variance was performed on the KDF 9 computer in the Computer Centre of the University of Birmingham using our own Fortran variance program. The program first computes, for each range
of truncation, $\sigma$, the position of the centroid (by iteration); it then computes the variance according to both the formulae

$$W(\sigma) = \int_{-\sigma}^{+\sigma} (\theta - \theta^*)^2 (\theta - \theta^*) d\theta$$

and

$$W'(\sigma) = \int_{-\sigma}^{+\sigma} (\theta - \theta^*)^2 (\theta - \theta^*) d\theta$$

Here $I(\theta)$ is the measured intensity distribution and $\sigma_{\text{max}}$ is the maximum range of truncation compatible with the measured set of intensities. [For the properties of $W(\sigma)$ and $W'(\sigma)$ see Wilson (1965a)]. In the next part of the program the variation of the variance in a predetermined range of $\sigma$ is expressed by means of the polynomial

$$W(\sigma) = \sum_{n=-6}^{n=0} a_n \sigma^n + b \log \sigma \quad (3)$$

The coefficients $a_n$ and $b$ are computed by the method of least squares. The number of terms in the polynomial can be adjusted by requiring the coefficients of the undesired terms to be zero. Output prints give the dependence of the centroid, of the integrated intensity and of the variance [both $W(\sigma)$ and $W'(\sigma)$] on the truncation range at equidistant steps from a predetermined minimum $\sigma_{\text{min}}$ to $\sigma_{\text{max}}$. The integrated intensity and the variance can be expressed either in angular units or in units of reciprocal space or in units of wavelength. (In the latter cases the influence of dispersion is not allowed for.) Finally the coefficients $a_n$ and $b$ are printed out together with the root-mean-square deviation of the values of variance computed from the polynomial with respect to the $W(\sigma)$.  

A separate part of the program computes the adjustments of the background level from the coefficient $a_3$ (and if required the adjustment of the slope of the background and/or its curvature from the coefficients $a_6$ and $a_9$ respectively). The method used here is based on the paper by Tourmarie (1956) and on the paper by Langford & Wilson (1963). Its successful application requires that all deviations of the variance in the truncation range from linearity be caused by inadequate setting of the level, slope or curvature of the background. The correction of some (or all three) background parameters and the subsequent recomputation of the variance-range function is repeated in three cycles in this program.

Finally an interpolation procedure is provided, enabling one to interpolate the diffraction profile in the region of the satellite group and to compute the variance function unaffected by its presence. The interpolation expresses the intensity of the diffraction profile by means of the polynomial

$$I(\theta) = \sum_{n=0}^{n=4} c_n (\theta_0 - \theta)^{-n}, \quad (4)$$

where $\theta_0$ is the coordinate of the peak of the $\alpha_1$ line. Coefficients $c_n$ are computed by the least-squares method from the intensity values in two intervals of adjustable width, situated on both sides of the interpolation interval. In Fig. 1 the interpolated profile is shown.

![Fig. 2. Variance-range functions for curves in Fig. 1. (a) Full curve: with satellite group; (b) dashed curve: satellite group removed by interpolation.](image-url)
In Fig. 2(a) the variance–range function $W(\sigma)$ is shown. The computation was performed on the intensity profile shown in Fig. 1 (measurement without the $\beta$ filter). The background level was taken from direct intensity measurements at points $\pm 11.5^\circ (2\theta)$ from the centroid. In this case computer interpolation of the background was not performed, for reasons discussed in § 4, nor was interpolation under the satellite group attempted.

The variance function exhibits two linear regions separated by the jump caused by the satellite group. The first and shorter linear part starts at about 5 mA and continues to 8 mA, where the influence of the satellite group starts to be pronounced. The second and longer linear part starts at about 12 mA and continues to $\sigma_{\text{max}}$, at about 24 mA. The slope of the first part is greater by $0.75 \times 10^{-4}$ A than the slope of the second part. It is important to know if this difference is caused by the deviation of the actual diffraction profile from the Cauchy form or if it is caused by the combined effect of the tail of the satellite jump and of the after-effect of the non-linear part of the variance function having its origin in the doublet form of the spectral distribution. To decide this, a computation of the variance by analytical integration was performed on an artificial doublet. Here the $\alpha_1$ line was approximated by two 'halves' of Cauchy functions each of maximum value 97.0. The half-width of the 'half' facing the high-energy side was 0.33 mA, the half-width of the low-energy 'half' was 0.53 mA. The maximum value and half-widths used to express the $\alpha_2$ line were 45.0, 0.44 and 0.55 mA respectively. The distance between $\alpha_1$ and $\alpha_2$ lines was taken as 3.93 mA. All these characteristics correspond to the actual profile in Fig. 1. The result of the computation is shown in Fig. 3. It must be stated that such an approximation to an asymmetric profile is just a mathematical convenience lacking any theoretical foundation. It represents the profile well at points not very distant from the central maxima but is expected to fail in the tails of the profile.

On the other hand, in this semi-quantitative discussion we can approximate the satellite group by a single rather wide Cauchy function (the satellite group was never fully resolved in our measurements) centred at 10 mA and with a half width of 2.7 mA. Its computed contributions to the slope are given in Table 1. Here $k_1$ is the derivative of the variance function corresponding to the $K\alpha_2$ doublet, $k_2$ is the derivative of the satellite contribution to the variance function and $k$ is the derivative of the resulting variance function. The quantity $k_1$ remains practically constant beyond 16 mA, so that we can consider this value as representing the slope in the region far beyond the satellite group and compare it with the slope in the region between 5 and 8 mA. Here the slope is also practically constant but this is caused merely by the mutual compensation of curvatures of the $K\alpha_2$ doublet contribution and of the satellite-group contribution to the total variance function. This computation shows that the slope in this first pseudolinear region is higher by about $0.5$ to $0.8 \times 10^{-4}$ A than in the linear part beyond the satellite group, which compares well with the result in Fig. 2(a), where the difference is $0.75 \times 10^{-4}$ A. This result suggests that, for the iron $K\alpha_2$ doublet, the variance function is truly linear only beyond the satellite group.

![Fig. 3. Variance–range function of an artificial doublet made up of halves of Cauchy functions.](image-url)
Table 1. Calculated slopes of \( W(\sigma) \) for an artificial doublet \((k_1)\), satellite group \((k_2)\) and their sum \((k)\), at various ranges

<table>
<thead>
<tr>
<th>( \sigma ) (mA)</th>
<th>( 10^{4} k_1 )</th>
<th>( 10^{4} k_2 )</th>
<th>( 10^{4} k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>3.72</td>
<td>0.04</td>
<td>3.76</td>
</tr>
<tr>
<td>6</td>
<td>3.45</td>
<td>0.12</td>
<td>3.57</td>
</tr>
<tr>
<td>7</td>
<td>3.29</td>
<td>0.30</td>
<td>3.59</td>
</tr>
<tr>
<td>8</td>
<td>3.20</td>
<td>0.68</td>
<td>3.88</td>
</tr>
<tr>
<td>10</td>
<td>3.12</td>
<td>2.53</td>
<td>5.65</td>
</tr>
<tr>
<td>12</td>
<td>3.08</td>
<td>0.86</td>
<td>3.94</td>
</tr>
<tr>
<td>14</td>
<td>3.05</td>
<td>0.26</td>
<td>3.31</td>
</tr>
<tr>
<td>16</td>
<td>3.03</td>
<td>0.06</td>
<td>3.09</td>
</tr>
<tr>
<td>18</td>
<td>3.02</td>
<td>0.02</td>
<td>3.04</td>
</tr>
</tbody>
</table>

Because of the satellite group, which extends to 12 mÅ, we must either start to consider the variance beginning with \( \sigma \geq 12 \) mÅ or we must remove the satellite group by interpolation. In our case the ratio of the intensity to background was rather bad (less than 2) for \( \sigma \geq 12 \) mÅ and therefore we adopted the interpolation procedure.

In Fig. 2(b) the variance function \( W(\sigma) \) of the same profile as in Fig. 2(a) is shown but with the satellite group removed by interpolation. The background level was taken from experiment without subsequent adjustment.

Table 2. Result of approximating \( W(\sigma) \) by a polynomial over an interval centred at \( A \) and of minimizing the coefficient \( a_3 \) to predict the correct background level \( B \)

<table>
<thead>
<tr>
<th>( A ) (mA)</th>
<th>( B )</th>
<th>Initial ( a_3 )</th>
<th>Final ( a_3 )</th>
<th>( 10^4 W'_0 ) (A)</th>
<th>( 10^4 k' ) (A)</th>
<th>( 10^6 W'_0 )</th>
<th>( 10^6 k' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>480</td>
<td>(-9.5 \times 10^{-2})</td>
<td>(1 \times 10^{-11})</td>
<td>2.85</td>
<td>2.40</td>
<td>1.84</td>
<td>2.78</td>
</tr>
<tr>
<td>13</td>
<td>746</td>
<td>(-0.4 \times 10^{-2})</td>
<td>(1 \times 10^{-3})</td>
<td>3.06</td>
<td>2.14</td>
<td>3.10</td>
<td>2.10</td>
</tr>
<tr>
<td>15</td>
<td>797</td>
<td>(1 \times 10^{-2})</td>
<td>(2 \times 10^{-9})</td>
<td>3.10</td>
<td>2.09</td>
<td>3.12</td>
<td>2.05</td>
</tr>
</tbody>
</table>

Fig. 4. Variance–range functions for different locations of the interval for expressing \( W(\sigma) \) as a polynomial. (a) Full curve: interval centre at 15 mÅ; (b) dashed curve: interval centre at 13 mÅ; (c) chain-dotted curve: interval centre at 11 mÅ.

4. The adjustment of the background

Tournarie (1956) and Langford & Wilson (1963) have shown that when the intensity distribution in the doublet can be expressed by Cauchy functions, an error in the level of the background gives a term proportional to \( \sigma^3 \) in the variance–range function and an error in the slope of background gives a term proportional to \( \sigma^4 \). Extending their computation by one additional term we can write

\[
W(\sigma) = W_0 + k\sigma + a_3\sigma^3 + a_5\sigma^5 + a_6\sigma^6, \tag{5}
\]

where

\[
a_3 = x/I, \quad a_5 = \frac{1}{2}x''/I \quad \text{and} \quad a_6 = \left(\frac{1}{2}\right)x'/I^2. \tag{6}
\]

Here \( x, x' \) and \( x'' \) are the errors in the level, first and second derivative of the background at the centroid, and \( I \) is the integrated intensity. This indicates a simple method for adjustment of the background level: we express the variance function by the polynomial (5) in the range where we can expect intrinsic linearity and from the coefficients \( a_3, a_5 \) and \( a_6 \) compute the required corrections. This method is inserted in the variance program in such a way that one can adjust either the level only, or firstly the level and in the next cycle the curvature, or firstly the level, then the curvature and finally the slope. This procedure has been applied to a
number of experimentally determined profiles with these results:

(i) It was virtually impossible to gain plausible results by refining parameters other than the level. Minor statistical fluctuations of intensity influence profoundly the partition of the non-linearity of the variance function between the terms \( \sigma^3 \), \( \sigma^5 \) and \( \sigma^6 \), and distort the corrections ascribed to the level, slope and curvature.

(ii) Even if we limit the polynomial to the form

\[
W(\sigma) = W + k\sigma + a_3\sigma^3
\]

and adjust only the level of the background, this method is useful only in the case where the profile is strictly inverse square and where we locate the range of \( \sigma \) over which the variance is approximated by the polynomial well clear of the initial part—in our case at least beyond 8 mA.

This point is demonstrated using the intensity distribution displayed in Fig. 1. We performed the computation of variance on this distribution with both the interpolation and adjustment of the level of the background. The length of the interval in which the variance was expressed by the polynomial (7) was the same in all runs but its centre was at 11 mA in the first run of computation, at 13 mA in the second and at 15 mA in the third. Each run consisted of 4 cycles in which the variance was recomputed and the level systematically readjusted to minimize the coefficient \( a_3 \). In Table 2 the final levels of background, the initial and final values of the coefficient \( a_3 \) and the intercept \( W_0 \) and the slope \( k' \) computed for \( \sigma = 10 \) mA and 15 mA for each of these three cases are shown.

We can observe how the adjusted level of background strongly depends on the location of the interval. The experimentally determined value of the background is 756. The variance functions corresponding to these three runs of computation are reproduced in Fig. 4.

In another series of computations the influence of mis-setting the slope of the background was tested. The computation was performed for different slopes and the width of the interval on which the computation of the coefficient \( a_3 \) was based was constant at 7 mA with its centre at 17.5 mA. This rather high value was used because the computation was performed without interpolation and the interval had to be placed well clear of the satellite-group jump. The results are given in Table 3.

<table>
<thead>
<tr>
<th>( C ) [counts/°(2θ)]</th>
<th>( 10^4k ) for ( \sigma = 15 ) mA</th>
<th>( B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-43</td>
<td>2.04</td>
<td>784</td>
</tr>
<tr>
<td>0</td>
<td>1.98</td>
<td>795</td>
</tr>
<tr>
<td>43</td>
<td>1.97</td>
<td>788</td>
</tr>
<tr>
<td>86</td>
<td>1.95</td>
<td>790</td>
</tr>
</tbody>
</table>

We can see that the change in the slope of the background has only a minute influence on the slope of the variance function. This confirms the observation by Langford & Wilson (1963). The applied change of the slope of the background corresponds to a change of the background from -300 impulses per 7°(2θ) to + 600 impulses per 7°(2θ). This exceeds by far the range of error likely to be met in practice. In our own measurement (Fig. 1) the slope of the background was 8 impulses /°(2θ).

Clearly, if experimentally one can obtain a reliable setting of the background, this should certainly be used in calculating the variance. If this is not possible, the above method of minimizing \( a_3 \) would be valuable; the dangers of this method have been indicated above and should be borne in mind.

5. Results

Table 4 summarizes the results and gives the values of intercepts and slopes for the variance function approximated as \( W_0 + k\sigma \). Table 4(a) collects results based on the measurements without a filter. In order to average out the minor deviations introduced by the computational technique, each value for \( \sigma = 10 \) mA was averaged from two computations with slightly different interpolation (based on slightly different ranges of fit and interpolation intervals); similarly, each value for \( \sigma = 15 \) mA was averaged from three computations, one without interpolation and two with interpolation. Table 4(b) gives results for the measurements with the filter, processed in the same way.

Table 4. Intercepts \( W_0 \), and slopes \( k \), of \( W(\sigma) \) for the Fe Kα doublet, according to the two definitions of \( W(\sigma) \) [equations (1) and (2)] at two different ranges

(a) Unfiltered radiation

<table>
<thead>
<tr>
<th>( \sigma ) (mA)</th>
<th>( 10^6W_0 ) (A°)</th>
<th>( 10^4k ) (A)</th>
<th>( 10^6W_0' ) (A°)</th>
<th>( 10^4k' ) (A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.24</td>
<td>1.95</td>
<td>3.13</td>
<td>2.00</td>
</tr>
<tr>
<td>15</td>
<td>3.13</td>
<td>2.03</td>
<td>3.06</td>
<td>2.06</td>
</tr>
</tbody>
</table>

(b) Filtered radiation

<table>
<thead>
<tr>
<th>( \sigma ) (mA)</th>
<th>( 10^6W_0 ) (A°)</th>
<th>( 10^4k ) (A)</th>
<th>( 10^6W_0' ) (A°)</th>
<th>( 10^4k' ) (A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.25</td>
<td>1.90</td>
<td>3.14</td>
<td>1.84</td>
</tr>
<tr>
<td>15</td>
<td>3.09</td>
<td>1.96</td>
<td>2.97</td>
<td>1.90</td>
</tr>
</tbody>
</table>

The background level for the intensity distribution without a filter was taken as the mean value of the intensity found at points ±11.5°(2θ) from the centroid. For the measurement with the β filter, the background level was computed on the assumption that the background levels corresponding to the measurements with and without filter (after subtracting the natural background) are proportional to the peak intensities in both measurements. In neither case was any background-level adjustment made.

For some applications the intercept and slope for the pseudolinear range are of interest. They are given in Table 5, where both \( W_0 \) and \( k \) refer to \( \sigma = 7 \) mA. The computation of variance was performed for the distribution of intensity with the satellite group.
Table 5. Intercepts, \(W_0\), and slopes, \(k\), of \(W(\sigma)\) in the pseudolinear region (at \(\sigma = 7\) mA), according to the two definitions of \(W(\sigma)\) [equations (1) and (2)]. Satellite group not interpolated.

<table>
<thead>
<tr>
<th>Definition 1</th>
<th>Definition 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10^6W_0)</td>
<td>(10^6W_0')</td>
</tr>
<tr>
<td>((\AA^2))</td>
<td>((\AA^2))</td>
</tr>
<tr>
<td>(10^6k)</td>
<td>(10^6k')</td>
</tr>
<tr>
<td>((\AA))</td>
<td>((\AA))</td>
</tr>
</tbody>
</table>

Without \(\beta\) filter: 2.74 2.69 2.46 2.90
With \(\beta\) filter: 2.73 2.66 2.45 2.86

The aberrations caused by slit dimensions and by the finite width of the crystal function are not very important. As will be shown elsewhere, the correction for the horizontal and vertical dimensions of the slits and \(W_\delta\) is the variance of the crystal function, expressed using the parameter \(y\) (Zachariasen, 1945),

\[ W_\sigma^{\text{corr}} = - \frac{1}{\tan\theta} \left[ \frac{\partial^2}{\partial \theta^2} W + \frac{\partial^2}{\partial y^2} W \right] + W_\sigma \]

where \(W_\sigma^{\text{corr}}\) is the variance corrected for aberrations, \(W_\sigma\) is the uncorrected variance, \(W_\epsilon\) and \(W_\delta\) represent the corrections for the horizontal and vertical dimensions of the slits and \(W_\epsilon\) is the variance of the crystal function, expressed using the parameter \(y\) (Zachariasen, 1945).

\( W_\epsilon, W_\delta\) and \(W_\epsilon\) are:

\[ W_\epsilon = \frac{1}{60} \frac{\Delta_1 + \Delta_2^2}{(d_1 + d_2)^2}, \quad W_\delta = \frac{\Delta^4}{80} \tan^2 \theta \]

and \(W_\epsilon\) is the half width of the slit limiting the primary beam, \(\Delta_1\) is the half width of the receiving slit, and \(d_1\) and \(d_2\) are their distances from the crystal and \(\Delta\) is the aperture of the Soller slit. Variance \(W_\epsilon\) was computed for a Darwinian profile.

In our case

\[ W_\epsilon = 1.4 \times 10^{-9} \text{rad}^2, \quad W_\delta = 1.8 \times 10^{-9} \text{rad}^2, \]

\( W_\epsilon \left( \frac{\partial^2}{\partial y^2} \right)^2 = 0.39 \times 10^{-10} + 0.35 \times 10^{-5} \sigma, \quad \text{and} \quad \left( \frac{\partial^2}{\partial \theta^2} \right)^2 = 0.62. \)

The sum of all aberrations is, therefore, \(2.0 \times 10^{-9} + 0.19 \times 10^{-5} \sigma [\text{Å}^2]\). The error in \(W_0\) is negligible; the error in \(k\), which amounts to \(0.02 \times 10^{-4} \text{Å}\) for \(\sigma = 10\) mA and \(0.03 \times 10^{-4} \text{Å}\) for \(\sigma = 15\) mA, was allowed for in Table 4.

The uncertainty in the background level causes an error which is more difficult to estimate. As can be inferred from Table 2, a displacement of the background level by 10 units changes the slope of the variance function by \(0.01 \times 10^{-4} \text{Å}\) for \(\sigma = 10\) mA and by \(0.02 \times 10^{-4} \text{Å}\) for \(\sigma = 15\) mA. We can expect that the background level was determined with an accuracy of \(\pm 20\) for the measurement without filter and \(\pm 50\) for the measurement with the filter. The influence of the level of the background on the intercept is slightly smaller. From Table 2 one can show that the change of background level by 10 changed the intercept by less than \(0.01 \times 10^{-4} \text{Å}^2\) for both \(\sigma = 10\) mA and \(\sigma = 15\) mA.

With respect to the lower accuracy of the background level for the measurement with the \(\beta\) filter it seems to be uncertain whether the differences between Tables 4 (a) and (b) are significant or not. A computation using the formula derived by Wilson (1965b) indicates that the effect of filtration is smaller than the expected errors in \(W_0\) and \(k\).

6. Conclusions

In this paper we have shown that the satellite group divides the variance–range function of the spectral distribution into two intervals, the 'pseudolinear' part before the satellite-group maximum and the true linear part beyond the satellite-group maximum. The slope of the pseudolinear part is greater than the slope of the linear part, and the reverse is true of the intercepts.

If the broadening function of the specimen is very narrow the form of the variance–range function is similar to that of the spectral distribution. Increasing the width of the broadening function of the specimen changes the form of the variance function; the step separating the pseudolinear and linear ranges merges gradually with the pseudolinear range. This behaviour, together with methods of correcting for the satellite group, will be considered in more detail in a later paper, but in summary we may note:

(i) If the variance–range function of the powder diffraction profile has been corrected for the effect of the satellite group, the use of the spectral variance function with the satellite group eliminated is appropriate (Table 4).

(ii) If the variance–range function of the powder diffraction profile has not been corrected for the effect of the satellite group, then the slope is too high and the intercept is too low. In this case the use of the spectral variance function based on the pseudolinear part (Table 5) gives a partial correction for the effect of the satellite group. The error, however, may be large in a certain range of diffraction broadening.

We are indebted to Professor A. J. C. Wilson for many helpful discussions and to the Science Research Council for a senior visiting fellowship (K. T.) and a maintenance grant (H. J. E.). The work was performed in the course of an investigation of metal powders of technical importance.

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